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A Computer Code for K- and L-Shell Ionization Cross Sections in the Plane-Wave Born Approximation

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A computer code DEKY has been written to calculate the K- and L-shell ionization cross sections by heavy charged-particle impact in the plane-wave Born approximation. Corrections for binding-energy and Coulomb-deflection effects as well as relativistic effect are taken into account.

KEY WORDS: K- and L-shell ionization cross section / Plane-wave Born approximation / Binding-energy, Coulomb-deflection, and relativistic effects /

I. INTRODUCTION

In recent years inner-shell ionization of atoms by impact of heavy charged particles, such as protons, α particles and carbon ions, has been studied both theoretically and experimentally. Extensive data on K- and L-shell ionization cross sections have been reported and theoretical cross sections have been calculated in the plane-wave Born approximation (PWBA).¹⁾

For low-velocity projectiles, two effects become important; (1) the increase in the binding energy of the target electron due to penetration of the projectile inside the inner shell during collision and (2) the deflection of the projectile by the Coulomb field of target nucleus. The PWBA theory modified for both effects has been successfully used to predict the direct Coulomb ionization cross sections. Furthermore, in the case of targets with large atomic number, the relativistic effect should be taken into consideration.

There have been already published numerical tables for the PWBA calculations,²⁻⁶⁾ and the ionization cross sections can be obtained from these tables by interpolation technique. However, it is useful to prepare a computer code to calculate ionization cross sections in the PWBA modified for the effects described above.

The computer code DEKY has been written to calculate the PWBA cross sections for K- and L-shell ionization by impact of heavy charged particles. The corrections for the binding-energy and Coulomb-deflection effects as well as the electronic relativistic effect are taken into account. The program has been written originally for the PDP-11/40 computer in the Institute of Nuclear Research of the Hungarian

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Academy of Sciences (ATOMKI) and then modified for the FACOM M-190 computer in the Data Processing Center of Kyoto University.

II. THEORY

A. Ionization Cross Section

The s -shell ionization cross section in the PWBA can be written as

$$\sigma_s = \frac{8\pi Z_1^2}{Z_s^4 \eta^2} f_s(\theta_s, \eta_s) a_0^2, \quad (1)$$

where $Z_1 e$ is the charge of the projectile, Z_s is the effective nuclear charge seen by the s -shell electron, and a_0 denotes the Bohr radius of the hydrogen.

When the projectile velocity is v_1 , the scaled projectile velocity parameter, η_s , is defined as

$$\eta_s = \frac{1}{Z_s^2} (h v_1 / e^2)^2, \quad (2)$$

and the scaled target-electron binding energy is given by

$$\theta_s = I_s n^2 / (Z_s^2 R_\infty), \quad (3)$$

where I_s is the measured ionization potential, R_∞ the Rydberg energy, and n is the principal quantum number of the s shell.

The function $f_s(\theta_s, \eta_s)$ is calculated as

$$f_s(\theta_s, \eta_s) = \int_{W_{\min}}^{W_{\max}} dW \int_{Q_{\min}}^{Q_{\max}} \frac{dQ}{Q^2} |F_{Ws}(Q)|^2, \quad (4)$$

where $Z_s Q^{1/2} / a_0$ is the momentum transfer and $W Z_s^2 R_\infty$ is the energy transfer. The lower limit of the integral with respect to W is taken to be $W_{\min} = \theta_s / n^2$, while $W_{\max} = (M_1/m) \eta_s$, where M_1 and m are the masses of the projectile and the target electron, respectively. On the other hand, Q_{\min} and Q_{\max} are given by:

$$Q_{\min} = (M_1/m)^2 \eta_s \{1 - [1 - mW / (M_1 \eta_s)]^{1/2}\}^2, \\ Q_{\max} = (M_1/m)^2 \eta_s \{1 + [1 - mW / (M_1 \eta_s)]^{1/2}\}^2.$$

The form factor, $F_{Ws}(Q)$, is given explicitly for K shell and each L subshell in Refs. 2 and 3.

B. Binding-Energy Effect

Basbas *et al.*⁷⁾ estimated the influence of the projectile on the initial state of the K-shell electron by the use of the perturbed-stationary-state theory. They incorporated this result in the PWBA and developed a simple method to include the effect of increased binding energy. According to them, the factor by which the scaled binding energy is increased is given by

$$\epsilon_s(\xi_s) = 1 + 2(Z_1 / Z_s \theta_s) g_s(\xi_s). \quad (5)$$

The parameter ξ_s is defined as

$$\xi_s = v_1 / \left(\frac{1}{2} \theta_s v_s \right), \quad (6)$$

where $v_s = Z_s v_0 / n$ and $v_0 = e^2 / \hbar$ is the Bohr velocity. The corresponding formula for L shell has been derived by Brandt and Lapicki.⁸⁾ The binding-energy effect can be taken into account by increasing θ_s to $\varepsilon_s \theta_s$.

The function $g_s(\xi_s)$ is estimated by the use of screened hydrogenic wave functions and by averaging the binding-energy increase over the impact-parameter-dependent ionization cross sections. The values are obtained by numerical integration and expressed in the analytical approximations:^{7,8)}

$$g_K(\xi) = (1 + 5\xi + 7.14\xi^2 + 4.27\xi^3 + 0.947\xi^4) / (1 + \xi)^5, \quad (7)$$

$$g_{L_1}(\xi) = (1 + 9\xi + 30.2\xi^2 + 66.8\xi^3 + 100\xi^4 + 94.1\xi^5 + 51.3\xi^6 + 15.2\xi^7 + 1.89\xi^8) / (1 + \xi)^9, \quad (8)$$

$$g_{L_{2,3}}(\xi) = (1 + 9\xi + 35.9\xi^2 + 84.5\xi^3 + 110\xi^4 + 91.9\xi^5 + 42.7\xi^6 + 12.2\xi^7 + 1.51\xi^8) / (1 + \xi)^9. \quad (9)$$

C. Coulomb Deflection

The Coulomb-deflection effect is taken into consideration through the method of Basbas *et al.*⁷⁾ They used the differential ionization cross section for hyperbolic trajectory of the projectile in the semiclassical approximation,^{9,10)} and derived a simple correction formula by integration over the energy transfer. The cross section with Coulomb-deflection effect, σ_s^C , can be expressed as

$$\sigma_{K,L_1}^C = 9E_{10}(\pi dq_0)\sigma_{K,L_1}^{PWBA}, \quad (10)$$

$$\sigma_{L_2,L_3}^C = 11E_{12}(\pi dq_0)\sigma_{L_2,L_3}^{PWBA}, \quad (11)$$

where $\hbar q_0$ is the minimum momentum transfer for ionization, d is the half-distance of closest approach in a head-on collision, $E_n(x)$ is the exponential integral of order n , and σ_s^{PWBA} denotes the PWBA cross section calculated from Eq. (1).

D. Relativistic Effect

The relativistic correction is incorporated through the usual method of Merzbacher and Lewis.¹⁾ The relativistic scaled binding energy is defined as

$$\theta_s^R = 1 - (I_s^R - I_s) / I_s^{NR}, \quad (12)$$

where I_s is the observed ionization potential, I_s^R the ionization energy for s shell calculated by the relativistic screened hydrogenic model, and I_s^{NR} that obtained from the nonrelativistic screened hydrogenic model. The relativistic cross sections are obtained from Eq. (1) by replacing θ_s of Eq. (3) by θ_s^R defined in Eq. (12).

III. DESCRIPTION OF THE PROGRAM

The program is designed to calculate the PWBA cross section, the PWBA modified for the binding-energy effect (PWBA-B), the PWBA-B including the Coulomb-deflection effect (PWBA-BC), and the PWBA-BC corrected for the relativistic effect

(PWBA-BCR).

Input for each case consists of two cards; a card for the projectile and a card for the target. After input data are read, the scaled binding energies, θ_s and θ_s^R , are determined. In the next step, the scaled projectile velocity, η_s , is estimated for a given projectile energy. Then the program starts to compute σ_s^{PWBA} . For this purpose, two subroutines are used. Subroutine F calculate the form factor $|F_{W_s}(Q)|^2$ for a fixed values of W and Q , and numerical integration over Q is performed in Subroutine FI. The numerical integration with respect to W is made and the cross section σ_s^{PWBA} is obtained from Eq. (1).

The binding-energy factor ϵ_s is estimated from Eq. (5) by using $g_s(\xi_s)$ function in Eqs. (7)~(9) and the scaled binding energy θ_s is replaced by $\epsilon_s\theta_s$. The procedures similar to those used for σ_s^{PWBA} are repeated and the PWBA-B cross section, $\sigma_s^{\text{PWBA-B}}$, is obtained. The factor for the Coulomb-deflection effect is determined from θ_s , ϵ_s , and η_s , and the PWBA-BC cross section is obtained by multiplying this factor to $\sigma_s^{\text{PWBA-B}}$.

Finally the relativistic correction is made. The scaled binding energy θ_s is replaced by θ_s^R of Eq. (12) and calculation of the cross section is made for $\epsilon_s\theta_s^R$. By multiplying the Coulomb-deflection factor, the PWBA cross section including binding-energy, Coulomb-deflection, and relativistic effects (PWBA-BCR) is obtained.

The projectile energy is increased by the energy step given in the input data and all the cross-section calculations are made for this energy. The whole procedures are repeated until the projectile energy exceed the maximum value given in the input. Then the program reads the next input cards.

IV. INPUT DATA SPECIFICATION

In the following we give details of the input required, including FORMAT specifications and explanations of the variables and options.

Card 1.	FORMAT (I10, F10.0, 2I5, F10.0)
IZ2	Atomic number of the target.
A2	Mass number of the target.
L	Identifying label for the atomic shell. For K shell $L=0$, and $L=i$ corresponds to L_i -shell electron.
N	Number of integration points. Usually 101.
BE	Measured binding energy of the target electron (keV).
Card 2.	FORMAT (2I5, 3F10.0)
IZ1	Atomic number of the projectile.
IA1	Mass number of the projectile.
EMIN	Minimum projectile energy (MeV).
EMAX	Maximum projectile energy (MeV).
DE	Energy step size (MeV).

A blank card will terminate the run or another input data may follow.

V. THE TEST RUN

The test run has been made for the K-shell ionization cross sections by protons on silver ($Z_2=47$). The energy range is taken to be between 0.5 and 1.0 MeV with the energy step of 0.5 MeV. Thus the cross sections are calculated for two projectile energies, 0.5 and 1.0 MeV.

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OUTPUT OF TEST RUN

```

***** TARGET *****
ATOMIC NUMBER = 47      MASS = 108
K SHELL      BINDING ENERGY = 25.514 KEV      INTEGRATION POINTS = 101

***** THETA = 0.86021E+00 *****

***** THETA (K) = 0.03116E+00 *****

***** PROJECTILE *****
ATOMIC NUMBER = 1      MASS = 1

***** NUMBER OF ENERGY POINTS 2 *****

*****
ENERGY = 0.50000E+00 MEV      YETA = 0.91017E-02

F-FUNCT      0.46547E-06

PWBA      0.75036E-26

GZAI      0.22279E+00
G      0.50104E+00
EPSIAUN      0.10459E+01
EPS-THE      0.09966E+00
F-FUNCT      0.31945E-06

PWBA-B      0.51474E-26

DEFLECT      0.27661E+00

PWBA-BC      0.19393E-26

***** RELATIVISTIC CORRECTION *****

GZAI      0.23057E+00
G      0.71094E+00
EPSIAUN      0.10472E+01
EPS-THE      0.07043E+00
F-FUNCT      0.42165E-06

PWBA-B      0.07972E-26

DEFLECT      0.36670E+00

PWBA-BC      0.06401E-26

*****
*****
ENERGY = 0.10000E+01 MEV      YETA = 0.10262E-01

F-FUNCT      0.11074E-04

PWBA      0.55710E-25

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GLAI	0.31507E+00
G	0.07101E+00
EPSIRON	0.10404E+01
EPS-THE	0.09753E+00
F-FUNCT	0.05725E-05

PRBA-B 0.69097E-25

DEFLECT 0.70790E+00

PRBA-UC 0.40914E-25

***** RELATIVISTIC CORRECTION *****

GLAI	0.22000E+00
G	0.00000E+00
EPSIRON	0.10446E+01
EPS-THE	0.00000E+00
F-FUNCT	0.11000E-04

PRBA-B 0.09171E-25

DEFLECT 0.71592E+00

PRBA-UC 0.00000E-25
